```
C:\stnweb\Queries\45.str
```

```
chain nodes :
    1 2 10 11 12 13 14 15 16 21 23 24 26

ring nodes :
    3 4 5 6 7 8

chain bonds :
    1-2 2-4 3-10 8-11 11-13 11-23 12-13 12-24 12-26 13-21

ring bonds :
    3-4 3-8 4-5 5-6 6-7 7-8

exact/norm bonds :
    1-2 2-4 3-4 3-8 3-10 4-5 5-6 6-7 7-8 8-11 11-13 11-23 12-13 12-24 12-26
    13-21
```

G1:0,S G2:[*1],[*2],[*3] G3:H,Ak

Match level:
1:Atom 2:CLASS 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 21:CLASS 23:CLASS 24:CLASS 26:CLASS

```
C:\stnweb\Queries\4.str
```

```
1 2 10 11 12 13 14 15 16 21 23 24 26 27 28 29 30 31 34 35 36 37 38
     42
ring nodes : 3 4 5 6 7 8
chain bonds:
     1-2 2-4 3-10 8-11 11-13 11-23 12-13 12-24 12-26 13-21 26-27 26-34 27-28 28-29
     28-30 30-31 34-42 35-36 37-38
ring bonds :
     3-4 3-8 4-5 5-6 6-7 7-8
exact/norm bonds:
1-2 2-4 3-4 3-8 3-10 4-5 5-6 6-7 7-8 8-11 11-13 11-23 12-13 12-24 12-26 13-21 28-29 28-30 30-31 34-42 35-36 37-38
exact bonds :
     26-27 26-34 27-28
G1:0,S
G2:[*1],[*2],[*3]
G3:H,Ak
G4:H,Cb,Ak,[*4],[*5]
Match level:
     1:Atom 2:CLASS 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 21:CLASS 23:CLASS 24:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 34:CLASS 35:Atom 36:CLASS 37:Atom
     38:CLASS 42:CLASS
```

chain nodes :

* * *	* *	* *	* *	* Welcome to STN International * * * * * * * * *									
NEWS	1			Web Page URLs for STN Seminar Schedule - N. America									
NEWS	2			"Ask CAS" for self-help around the clock									
NEWS		SEP	09	CA/CAplus records now contain indexing from 1907 to the									
				present									
NEWS		DEC		INPADOC: Legal Status data reloaded									
NEWS		SEP		DISSABS now available on STN									
NEWS		OCT		PCTFULL: Two new display fields added									
NEWS		OCT		BIOSIS file reloaded and enhanced									
NEWS		OCT		BIOSIS file segment of TOXCENTER reloaded and enhanced									
NEWS		NOV		MSDS-CCOHS file reloaded									
NEWS		DEC		CABA reloaded with left truncation									
NEWS		DEC		IMS file names changed									
NEWS	12	DEC	09	Experimental property data collected by CAS now available in REGISTRY									
NEWS	13	DEC	09	STN Entry Date available for display in REGISTRY and CA/CAplus									
NEWS	14	DEC	17	DGENE: Two new display fields added									
NEWS	15	DEC	18	BIOTECHNO no longer updated									
NEWS	16	DEC	19	CROPU no longer updated; subscriber discount no longer									
				available									
NEWS	<u>17</u>	DEC	22	Additional INPI reactions and pre-1907 documents added to CAS									
				databases									
NEWS		DEC		IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields									
NEWS		DEC		ABI-INFORM now available on STN									
NEWS	20	JAN	27	Source of Registration (SR) information in REGISTRY updated									
				and searchable									
NEWS	21	JAN	27	A new search aid, the Company Name Thesaurus, available in									
MEMO	22	מממ	ΛE	CA/CAplus German (DE) application and patent publication number format									
NEWS	22	FEB	US	changes									
NEWS	23	MAR	03	MEDLINE and LMEDLINE reloaded									
NEWS		MAR		MEDLINE file segment of TOXCENTER reloaded									
NEWS		MAR		FRANCEPAT now available on STN									
пано			0.5										
NEWS	EXP	RESS	MA	RCH 5 CURRENT WINDOWS VERSION IS V7.00A, CURRENT									
			MA	CINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),									
		AN.	AND CURRENT DISCOVER FILE IS DATED 3 MARCH 2004										
NEWS HOURS			ST	N Operating Hours Plus Help Desk Availability									
			Ge:	eneral Internet Information									
NEWS	LOG	IN		lcome Banner and News Items									
NEWS	PHO	NE		irect Dial and Telecommunication Network Access to STN									
NEWS	WWW		CA	S World Wide Web Site (general information)									

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 15:08:44 ON 21 MAR 2004

=> file reg COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 15:08:50 ON 21 MAR 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 MAR 2004 HIGHEST RN 665776-10-3 DICTIONARY FILE UPDATES: 19 MAR 2004 HIGHEST RN 665776-10-3

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP_PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> L1

STRUCTURE UPLOADED

=> 13

L1 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> d 11

L1 HAS NO ANSWERS

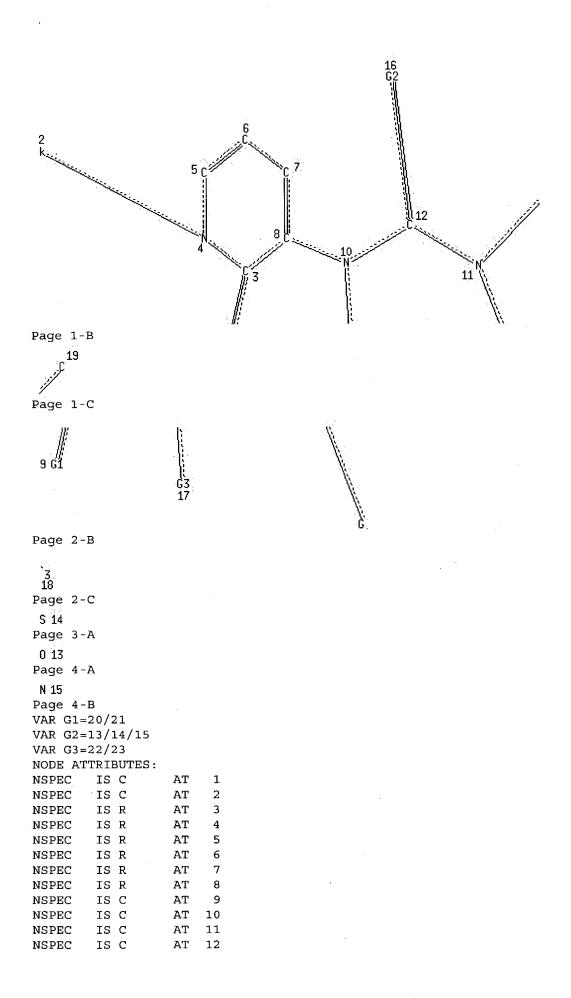
L1 STR

H 22 Ak 23

0 20 S 21

2 1 Cb -------A

Page 1-A



```
IS C
                 AT 13
NSPEC
NSPEC IS C
                  AT 14
NSPEC IS C
                  AT 15
NSPEC
      IS C
                  AΤ
                     16
       IS C
                  AT
                     17
NSPEC
        IS C
                      18
NSPEC
                  AT
        IS C
                  ΑT
                      19
NSPEC
DEFAULT MLEVEL IS ATOM
                     2 10 11 12 13 14 15 19 20 21 22 23
MLEVEL IS CLASS AT
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 23
STEREO ATTRIBUTES: NONE
=> s 11
SAMPLE SEARCH INITIATED 15:12:21 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 105 TO ITERATE
100.0% PROCESSED
                     105 ITERATIONS
                                                              19 ANSWERS
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS:
                        ONLINE **COMPLETE**
                               **COMPLETE**
                        BATCH
                              1486 TO
PROJECTED ITERATIONS:
                                          2714
PROJECTED ANSWERS:
                               119 TO
                                           641
             19 SEA SSS SAM L1
L2
=> s 11 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y) /N or END:y
FULL SEARCH INITIATED 15:12:26 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -
                                 2405 TO ITERATE
                                                              563 ANSWERS
100.0% PROCESSED
                    2405 ITERATIONS
SEARCH TIME: 00.00.01
            563 SEA SSS FUL L1
L3
=>
        STRUCTURE UPLOADED
L4
L4 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).
=> d 14
L4 HAS NO ANSWERS
L4
                STR
```

H 37 Cb 389k 39

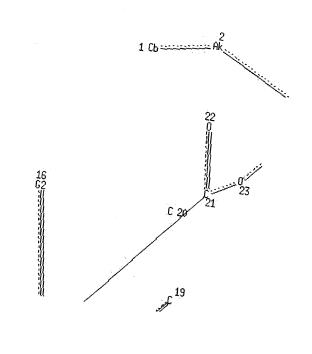
H 35 Ak 36

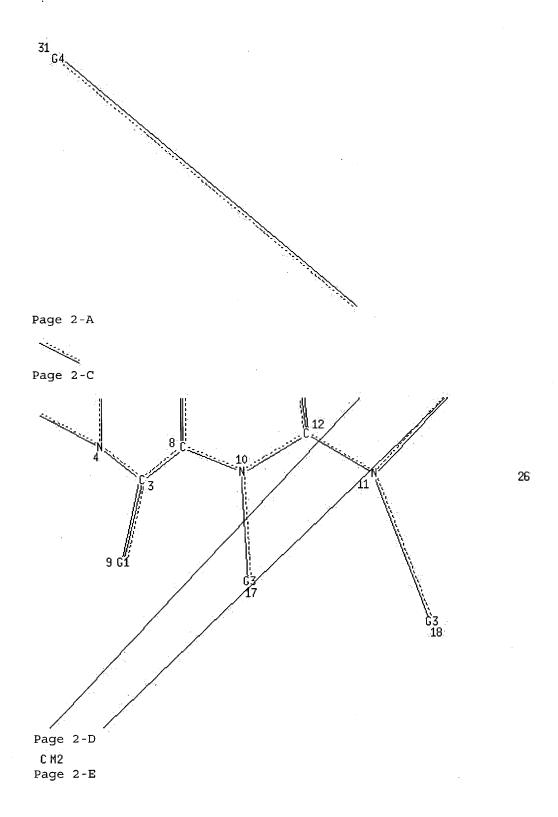
0 33 S 34

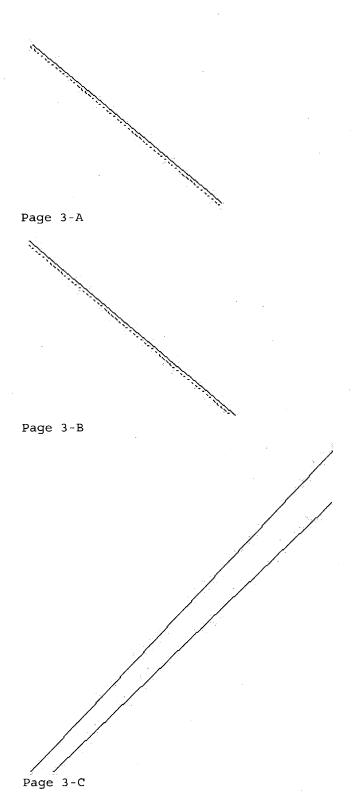


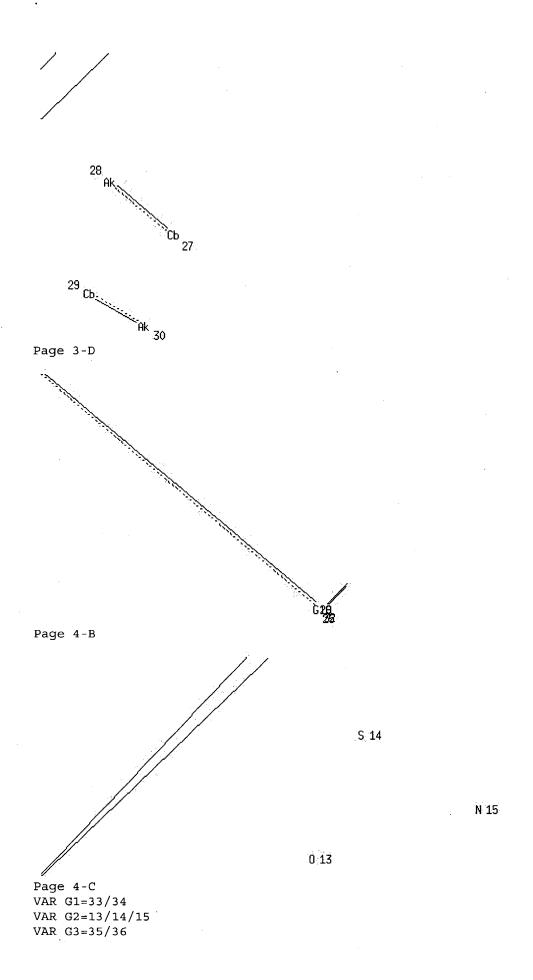


Page 1-E









```
IS C
NSPEC
                 AT
       IS R
                 AT
NSPEC
                       3
       IS R
                 AT
NSPEC
                       4
      IS R
                 AT
                       5
NSPEC
NSPEC
       IS R
                 AT
NSPEC
       IS R
                 AT
                       7
       IS R
                 AT
NSPEC
                       8
       IS C
NSPEC
                 AT
                      9
NSPEC
       IS C
                 AT
                     10
NSPEC
       IS C
                 AT
                     11
NSPEC
      IS C
                 AT
                     12
NSPEC
      IS C
                 AT
                     13
NSPEC
       IS C
                 AT
                     14
       IS C
NSPEC
                 AT
                     15
NSPEC
       IS C
                 AT
                     16
NSPEC
       IS C
                 \mathbf{AT}
                     17
NSPEC
       IS C
                 AT
                     18
NSPEC
      IS C
                 AT
                     19 -
      IS C
                 AT
                     20
NSPEC
NSPEC
      IS C
                 AT
                     21
NSPEC
       IS C
                 AT
                     22
                 AT
NSPEC
       IS C
                     23
                 ΑT
NSPEC
       IS C
NSPEC
       IS C
                 AT
                     25
               AT
NSPEC
      IS C
                     26
NSPEC
      IS C
                 AT 27
NSPEC
       IS C
                 AT
                     28
NSPEC
       IS C
                 AT
                     29
       ÍS C
NSPEC
                 AT
                     30
NSPEC
       IS C
                  AΤ
                     31
       IS C
NSPEC
                  AT
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT
                       2 10 11 12 13 14 15 19 20 21 22 23 26 28 30 33 34
          35 36 37 38 39
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 39
STEREO ATTRIBUTES: NONE
=> $ 14
SAMPLE SEARCH INITIATED 15:16:58 FILE 'REGISTRY'
                                   42 TO ITERATE
SAMPLE SCREEN SEARCH COMPLETED -
                                                              19 ANSWERS
100.0% PROCESSED
                      42 ITERATIONS
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                                **COMPLETE**
                        BATCH
PROJECTED ITERATIONS:
                               452 TO
                                          1228
PROJECTED ANSWERS:
                               119 TO
                                           641
```

VAR G4=37/38/39/28/29 REP G19=(0-3) 26-19 26-31 REP G20=(1-2) 20-19 20-21

IS C

AΤ

AT

26

1

NODE ATTRIBUTES: HCOUNT IS M2

NSPEC

19 SEA SSS SAM L4

=> s 14 full

L5

L6

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 15:17:03 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1062 TO ITERATE

100.0% PROCESSED 1062 ITERATIONS

554 ANSWERS

SEARCH TIME: 00.00.01

554 SEA SSS FUL L4

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

315.88

316.09

FILE 'HCAPLUS' ENTERED AT 15:17:07 ON 21 MAR 2004
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FILE COVERS 1907 - 21 Mar 2004 VOL 140 ISS 13 FILE LAST UPDATED: 19 Mar 2004 (20040319/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 16

L7

2 L6

=> d 17, ibib abs fhitstr, 1-2

L7 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER:

2002:349146 HCAPLUS

DOCUMENT NUMBER:

136:369608

TITLE:

Preparation of 3-(N'-oxodihydropyridinylureido)-3-

phenylpropanoates as inhibitors of $\alpha 4\beta 1$

integrin binding

INVENTOR(S):

Biediger, Ronald J.; Chen, Qi; Holland, George W.; Kassir, Jamal M.; Li, Wen; Market, Robert V.; Scott,

Ian L.; Wu, Chengde; Decker, Radford E.; Li, Jian

PATENT ASSIGNEE(S):

Texas Biotechnology Corporation, USA

SOURCE:

Eur. Pat. Appl., 131 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent English

LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

]	PATENT	KIND DATE				APPLICATION NO.					DATE						
									-								
]	EP 1203766			A2 20020508			EP 2001-125494						20011106				
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR	, IT,	LI,	LU,	NL,	SE,	MC,	PT,
		IE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL	, TR						
<u>;</u>	ZA 2001	10087	77	Α		2003	0124		<u>Z</u> .	A 2	001-8	3777		2001	1024		
]	NO 2001	10053	94	Α		2002	0507		N	0 2	001-5	394		2001	1105		
(CN 1412	2181		Α		2003	0423		C	N 2	001-1	4518	2	2001	1229		
	JP 2003	31191	81	A2	2	2003	0423		J	P 2	002-3	1953		2002	0208		
PRIOR	ITY API	PLN.	INFO	. :				1	US 2	000	-7070)68	Α	2000	1106		
								1	115 2	001	-9731	42	Δ	2001	1009		

OTHER SOURCE(S):

MARPAT 136:369608

AB Title compds. were prepd. Thus, 2-ClC6H4CH2ZNH2 (Z = 4-ethyl-2-oxo-1,2-dihydropyridine-1,3-diyl) (prepn. given) was condensed with

(S)-4-MeC6H4CH(NH2)CH2CO2Et and COCl2 to give, after sapon.,

(S)-2-ClC6H4CH2ZNHCONHCH(C6H4Me-4)CH2CO2H (Z as above). Data for biol. activity of title compds. were given.

IT 307520-20-3P

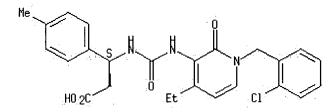
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 3-(N'-oxodihydropyridinylureido)-3-phenylpropanoates as inhibitors of $\alpha 4\beta 1$ integrin binding)

RN 307520-20-3 HCAPLUS

CN Benzenepropanoic acid, β -[[[[1-[(2-chlorophenyl)methyl]-4-ethyl-1,2-dihydro-2-oxo-3-pyridinyl]amino]carbonyl]amino]-4-methyl-, (β S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References
ACCESSION NUMBER:

2000:814302 HCAPLUS

DOCUMENT NUMBER:

133:362963

TITLE:

Preparation of β -amino acid derivatives that

inhibit the binding of integrins to their receptors Biediger, Ronald J.; Chen, Qi; Holland, George W.;

Kassir, Jamal M.; Li, Wen; Market, Robert V.; Scott,

Ian L.; Wu, Chengde

PATENT ASSIGNEE(S):

Texas Biotechnology Corporation, USA

SOURCE:

PCT Int. Appl., 113 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

INVENTOR(S):

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

	PATENT NO.			KI	ND :	D DATE APPLICATION NO. DATE													
	WO 2000067746				A1 20001116				WO 2000-US12303						20000505				
	WO 2000067746			46	C2 20020829														
		W:	ΑE,	AL,	AM,	ΑT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CR,	CU,	
			CZ,	DE,	DK,	DM,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	HU,	ID,	IL,	
			IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MA,	
			MD,	MG,	MK,	MN,	MW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	
			SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VN,	YU,	ZA,	ZW,	AM,	
			ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM									
		RW:	GH,	GM,	KE,	LS,	MW,	SD,	SL,	SZ,	TZ,	UG,	ZW,	ΑT,	BE,	CH,	CY,	DE,	
			DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	
			CG,	CI,	CM,	GA,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG					
	EP 1176956			A	1	2002	0206		EP 2000-937527 20000505										
		R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
			ΙE,	SI,	LT,	LV,	FI,	RO											
	SI 2	0744	<u> </u>		C		2002	0630		S	I 20	00-2	0021		2000	0505			
	BR 2	0000	102	93	A 20020716			BR 2000-10293						20000505					
															2000				
	ZA 2	0010	087	74	Α		2003	0124		Z	A 20	01-8	774	_	2001	1024			
	NO 2	0010	054	18	Α		2001	1221		No	20	01-54	418		2001	1106			
PRIO	PRIORITY APPLN. INFO				.:				US 1999-132971P P					P	19990507				
WO 2000-US12303 W 20000505																			
OTHE	OTHER SOURCE(S): MARPAT 133:362963																		
GI				•															

AB Title compds. I [Y, at each occurrence, independently = CO, N, CR1, CR2R3, NR5, CH, O, or S; q = 3-10; A = O, S, CR16R17, NR6; E = CH2, O, S, NR7; J = O, S, NR8; M = CR9R10 or (CH2)0-3; T = CO or (CH2)0-3; L = O, NR11, S, (CH2)0-1; X = CO2B, PO3H2, SO3H, SO2NH2, SO2NHCOR12, OPO3H2, CONHCOR13, CONHSO2R14, tetrazolyl, hydroxyl, H; W = C, CR15, N; B, R1-17 = H, halo, hydroxyl, alkyl, alkoxy, aliph. acyl, CF3, nitro, cycloalkyl, alkylheteroaryl, sulfonyl, carboxyl, etc.] or their pharmaceutically acceptable salts were prepd. for inhibition of the binding of $\alpha 4\beta 1$ integrin to its receptors. Thus, II was prepd. and assayed (IC50 = 0.2 μ M) for its ability to suppress binding using a 26-amino acid peptide contg. the CS-1 sequence of fibronectin with N-terminal cysteine coupled to maleimide activated ovalbumin.

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of β -amino acid derivs. that inhibit the binding of integrins to their receptors)

RN 307520-20-3 HCAPLUS

CN Benzenepropanoic acid, β -[[[[1-[(2-chlorophenyl)methyl]-4-ethyl-1,2-dihydro-2-oxo-3-pyridinyl]amino]carbonyl]amino]-4-methyl-, (β S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

3

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold				
COST IN U.S. DOLLARS	SINCE FILE	TOTAL		
	ENTRY	SESSION		
FULL ESTIMATED COST	11.87	327.96		
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL		
	ENTRY	SESSION		
CA SUBSCRIBER PRICE	-1.39	-1.39		

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FILE COVERS 1907-1966 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter <u>HELP FIRST</u> for more information.

=> d his

(FILE 'HOME' ENTERED AT 15:08:44 ON 21 MAR 2004)

FILE 'REGISTRY' ENTERED AT 15:08:50 ON 21 MAR 2004

L1 STRUCTURE UPLOADED

L2 19 S L1

L3 563 S L1 FULL

L4 STRUCTURE UPLOADED

L5 19 S L4

L6 554 S L4 FULL

FILE 'HCAPLUS' ENTERED AT 15:17:07 ON 21 MAR 2004

L7 2 S L6

FILE 'CAOLD' ENTERED AT 15:17:24 ON 21 MAR 2004

=> s 16

L8 0 L6

=> log y

COST IN U.S. DOLLARS SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST 0.42 328.38

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

ENTRY SESSION

CA SUBSCRIBER PRICE 0.00 -1.39

STN INTERNATIONAL LOGOFF AT 15:17:37 ON 21 MAR 2004